

1,1,2,2-Tetrafluoro-2-(1,2,2,2-tetrafluoroethoxy)ethane-1-sulfonyl fluoride
446312-61-4 | DTXSID00580271

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.16

Global applicability domain: Inside

Local applicability domain index: 4.28e-01

Confidence level: 6.86e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Moxisylyte</div> <div>Measured: 3.17</div> <div>Predicted: 3.14</div>	<div>Image not found</div> <div>Deacetylmoxisylyte</div> <div>Measured: 2.93</div> <div>Predicted: 3.17</div>
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